Quantum Phase Transition in the Sub-Ohmic Spin-Boson Model: Extended Coherent-state Approach

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We propose a general extended coherent state approach to the qubit (or fermion) and multi-mode boson coupling systems. The application to the spin-boson model with the discretization of a bosonic bath with arbitrary continuous spectral density is described in detail, and very accurate solutions can be obtained. The quantum phase transition in the nontrivial sub-Ohmic case can be located by the fidelity and the order-parameter critical exponents for the bath exponents $s < 1/2$ can be correctly given by the fidelity susceptibility, demonstrating the strength of the approach.

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The spin-boson model [1, 2] describes a qubit (two-level system) interacting with an infinite collection of harmonic oscillators that models the environment acting as a dissipative bosonic "bath". There are currently considerable interests in this quantum many-body system due to the rich physics of quantum criticality and decoherence [3–5], applied to the emerging field of quantum computations, quantum devices [6], and biology [7, 8]. The dissipative environment [9] in the spin-boson model is characterized by the spectral function $J(\omega)$ with frequency behavior $J(\omega) \propto \omega^s$. The spin-boson model undergoes a second-order quantum phase transitions (QPT) from delocalized to localized phase with a sub-Ohmic bath ($0 < s < 1$) and a Kosterlitz-Thouless type transition in the Ohmic case ($s = 1$).

To provide reliable solutions for the spin-boson model, a typical multi-mode system, is quite challenging. Although several numerical methods applied to the sub-Ohmic case[10, 11, 13–16, 18] can reproduce the phase diagram, only recent quantum Monte Carlo (QMC) simulations [15] and exact-diagonalization studies [16] are capable of correctly extracting the critical exponents in the QPT. The critical behavior in the previous standard numerical renormalization group (NRG) calculations [10, 11, 18] is incompatible with a mean-field transition due to the failure of the quantum-to-classical mapping with long-range interactions for $s < \frac{1}{2}$. More recently, the early standard NRG results were improved by a modified NRG algorithm[17], and the mean-field behavior for $s < 1/2$ was also reproduced.

In this paper, we present a general accurate approach to the qubit (or fermion) and multi-mode boson coupling systems. As a important example, we focus on the sub-ohmic spin-boson model here. It can also be easily extended to the famous Holstein model[19] and the multi-mode Dicke model[20]. The crucial procedure is to employ extended coherent states to represent the bosonic states. The QPT in the sub-ohmic spin-boson model will be analyzed by means of the quantum information tools, such as the ground state fidelity and fidelity susceptibility [21–23]. It is a great advantage to use the fidelity to characterize the QPT, since there should be a dramatic change in the fidelity across the critical points. Moreover, the non-trivial order-parameter critical exponents can be obtained with scaling of the fidelity susceptibility.

The Hamiltonian of the spin-boson model is given by

$$H = -\frac{\Delta}{2}\sigma_x + \frac{\epsilon}{2}\sigma_z + \sum_n \omega_n a_n^\dagger a_n + \frac{1}{2}\sigma_z \sum_n \lambda_n (a_n^\dagger + a_n), \tag{1}$$

where σ_x and σ_z are Pauli matrices, Δ is the tunneling amplitude between two levels, ω_n and $a_n^\dagger$ are the frequency and creation operator of the n-th harmonic oscillator, and λ_n is the coupling strength between the n-th oscillator and the local spin. The spin-boson coupling is characterized by the spectral function,

$$J(\omega) = \pi \sum_n \lambda_n^2 \delta(\omega_n - \omega) = 2\pi\alpha\omega_c^{1-s}\omega^s, 0 < \omega < \omega_c \tag{2}$$

with ω_c a cutoff frequency. The dimensionless parameter α denotes the strength of the dissipation. $s = 1$ stands for an Ohmic dissipation bath. The rich physics of the quantum dissipation is second-order QPT from delocalization to localization for $0 < s < 1$, as a consequence of the competition between the amplitude of tunneling of the spin and the effect of the dissipative bath.

We here propose a solution of the spin-boson model by exact diagonalization in the coherent-states space. To implement our approach, we first perform discretization of the bath speciation function, according to the logarithmic discretization of the continuous spectral density $J(\omega)$ in the NRG [10, 11, 18]. The discrete Hamiltonian is therefore expressed as

$$H_n = -\frac{\Delta}{2}\sigma_x + \frac{\epsilon}{2}\sigma_z + \sum_n \xi_n a_n^+ a_n + \frac{\sigma_z}{2\sqrt{\pi}} \sum_n \gamma_n (a_n^+ + a_n) \tag{3}$$

with

$$\xi_n = \gamma_n^{-2} \int_{\Lambda^{-(n+1)}\omega_c}^{\Lambda^{-n}\omega_c} dx J(x) x, \gamma_n^2 = \int_{\Lambda^{-(n+1)}\omega_c}^{\Lambda^{-n}\omega_c} dx J(x) \tag{4}$$

In order to ensure the convergence of the results, the disctetiztion parameter is chosen $\Lambda = 2$.

The present basic scheme is similar to that in the single-mode Dicke model [25] and the two-site Holstein-Hubbard model [26]. For convenience, we assume that $|\varphi_1\rangle$ and $|\varphi_2\rangle$ are the bosonic states corresponding to spin up and down. Introducing a displacement shift parameter $g_n = \frac{\gamma_n}{2\xi_n\sqrt{\pi}}$ [18], we propose the following two coherent bosonic operators

$$A_n^+ = a_n^+ + g_n, A_n = a_n + g_n \tag{5}$$
$$B_n^+ = a_n^+ - g_n, B_n = a_n - g_n. \tag{6}$$

The corresponding vacuum states $|0\rangle_{A_n}$ and $|0\rangle_{B_n}$ are just the coherent states in a_n with eigenvalues $\mp g_n$ in terms of $e^{\mp g_n a^+ - g_n^2/2}|0\rangle_{a_n}$. $|n_k\rangle_{A_k}$ and $|n_k\rangle_{B_k}$ correspond to Fock states of the new bosonic operators A_k^+ and B_k^+ with n_k bosons for a frequency ω_k. $|\varphi_1\rangle$ and $|\varphi_2\rangle$ can be expanded in the bosonic coherent states of a series of n_k, which are orthonormalized in the new bosonic operators $A_k^+(B_k^+)$

$$|\varphi_1\rangle = \sum_{n_1...n_N}^{N_{tr}} c_{n_1...n_N} \prod_{k=1}^{N} |n_k\rangle_{A_k}, \tag{7}$$
$$|\varphi_2\rangle = \sum_{n_1...n_N}^{N_{tr}} d_{n_1...n_N} \prod_{k=1}^{N} |n_k\rangle_{B_k} \tag{8}$$

where $c'_{\{n_k\}}$ are coefficients with respect to a series of $\{n_1, n_2...n_N\}$ for different bosonic modes, and N_{tr} is the bosonic truncated number.

Then the Schrödinger equations of the Hamiltonian (3) are derived as

$$-\frac{\Delta}{2}|\varphi_2\rangle - \frac{\epsilon}{2}|\varphi_1\rangle + \sum_{n=0}^{\infty} \xi_n(A_n^+ A_n - g_n^2)|\varphi_1\rangle = E|\varphi_1\rangle \tag{9}$$
$$-\frac{\Delta}{2}|\varphi_1\rangle + \frac{\epsilon}{2}|\varphi_2\rangle + \sum_{n=0}^{\infty} \xi_n(B_n^+ B_n - g_n^2)|\varphi_2\rangle = E|\varphi_2\rangle \tag{10}$$

After the substitution of Eqs. (7) and (8) and Left multiplying the bosonic coherent states with the both sides of Eqs. (9) and (10), we have

$$\sum_{i=0}^{\infty} \xi_i(m_i - g_i^2) c_{\{m_k\}} - \frac{\Delta}{2} \sum_{\{n_k\}} d_{\{n_k\}} \prod_{k=1}^{N} {}_{A_k}\langle m_k|n_k\rangle_{B_k} - \frac{\epsilon}{2} c_{\{m_k\}} = E c_{\{m_k\}}, \tag{11}$$

$$\sum_{i=0}^{\infty} \xi_i(m_i - g_i^2) d_{\{m_k\}} - \frac{\Delta}{2} \sum_{\{n_k\}} c_{\{n_k\}} \prod_{k=1}^{N} {}_{B_k}\langle m_k|n_k\rangle_{A_k} + \frac{\epsilon}{2} d_{\{m_k\}} = E d_{\{m_k\}} \tag{12}$$

The bosons state $|n_k\rangle$ and $|m_k\rangle$ with different coherent bosonic operators A_k^+ and B_k^+ are not orthogonal. The overlap can be denoted by ${}_{A_k}\langle m_k|n_k\rangle_{B_k} = (-1)^{n_k} D_{m_k n_k}$ and ${}_{B_k}\langle m_k|n_k\rangle_{A_k} = (-1)^{m_k} D_{m_k n_k}$ with

$$D_{m_k n_k} = e^{-2g_k^2} \sum_{i=0}^{\min\{m_k,n_k\}} (-1)^i \frac{\sqrt{m_k! n_k!}(2g_k)^{m_k+n_k-2i}}{i!(m_k-i)!(n_k-i)!}.$$

According to the symmetry of Hamiltonian for $\epsilon = 0$, the coefficients satisfy $c_{m_1...m_N} = \pm(-1)^{\sum_k m_k} d_{m_1...m_N}$. Eqs.(11) and (12) can then be transformed into the following set of coupled equations

$$\mp\frac{\Delta}{2} \sum_{n_1...n_N} c_{\{n_k\}} \prod_{k=1}^{} D_{m_k n_k} + \sum_{i=0}^{\infty} \xi_i(m_i - g_i^2) c_{\{m_k\}} = E c_{\{m_k\}} \tag{13}$$

A complete implementation of the numerical diagonalization is described below to obtain the amplitudes set of $c_{\{n_k\}}$ of the bosonic state φ_1 (φ_2). The Hilbert space can be labeled by a vector $\overrightarrow{n} = (n_1, ..., n_N)$ with $n_k = 0, 1, ..., N_{tr}$. The sum of bosonic number n_k is restricted to truncated number N_{tr}, e.g. $\sum n_k \le N_{tr}$. For example, with a set of $N = 3, N_{tr} = 3$ the involved configurations of bosonic states $|n_1, n_2, n_3>$ are expressed as following:

$$|000\rangle,$$

$$|100\rangle, |010\rangle, |001\rangle,$$

$$|200\rangle, |110\rangle, |020\rangle, |101\rangle, |011\rangle, |002\rangle,$$

$$|300\rangle, |210\rangle, |120\rangle, |030\rangle, |201\rangle, |111\rangle, |021\rangle, |102\rangle, |012\rangle, |003\rangle.$$

Consequently, the total number of basis states $N_s = 20$. To obtain the true exact results, in principle, the number of bosonic modes N and the truncated number N_{tr} should be taken to infinity. Fortunately, in the present calculation, setting $N = 16$, which is big enough in NRG, and $N_{tr} = 5$ is sufficient to give very accurate results with relative errors less than 10^{-5} in the whole parameter space. The following results are just obtained with $N = 16$ and $N_{tr} = 5$.

To study the QPT in the sub-Ohmic spin-boson model, we employ the ground state fidelity to locate the critical point α_c. A simple expression of the ground-state fidelity is given just by the modulus of the overlap

$$F(\alpha, \alpha') = |\langle\varphi_1(\alpha)|\varphi_1(\alpha')\rangle + \langle\varphi_2(\alpha)|\varphi_2(\alpha')\rangle| \tag{14}$$

The QPT is expected to be signaled by a drop in the fidelity corresponding to two arbitrarily neighboring Hamiltonian parameters $\alpha' = \alpha + \delta\alpha$ [21, 23]. Based on the normalized ground states $|\varphi_1\rangle$ and $|\varphi_2\rangle$, we now illustrate our results obtained by numerically diagonalization of Eq.(13).

Fig. 1 (a) shows the behavior the fidelity $F(\alpha,\alpha')$ in the sub-Ohmic case with $s = 0.5, 0.6, 0.8, 0.9$ for the spin tunneling amplitude $\Delta = 0.01$. A sharp drop at the critical point α_c separates the delocalized phase at small α and the localized phase at large α. So it is evident that we can locate the critical points α_c efficiently by the ground state fidelity. It is interesting that the ground state fidelity does not drop to 0 at critical points, demonstrating a continuous QPT[24].

The QPT from delocalized to localized phases can also be shown by behavior of the tunneling motion $\langle\sigma_x\rangle$ between spin up and spin down [13]. $\langle\sigma_x\rangle$ goes rapidly to zero in the localized phase and is finite in the delocalized phase. The $\alpha(\Delta, s)$ dependence of $\langle\sigma_x\rangle$ is shown in Fig. 1(b). For all value of s, we observe that $\langle\sigma_x\rangle$ is continuous at the transition. The discontinuous behavior observed previously [13] may be attributed to the special variational approach itself, and is perhaps worthy of a further study.

As discussed above, both the fidelity $F(\alpha,\alpha')$ and tunneling parameter $\langle\sigma_x\rangle$ can be used to locate the critical points of the QPT. We observe that both quantities can give nearly the same critical points. The phase boundaries obtained by either methods as a function of s is plotted in Fig. 2 in case of the tunnel splitting Δ ranging from 10^{-4} to 10^{-1} for $\epsilon = 0$. The results from previous NRG techniques[10, 11] are also collected for comparison. It is interesting to note that the present results for the critical points are in good agreement with the NRG ones. Because we also use the truncated NRG Hamiltonian (3), the critical points should be slightly above the QMC ones[15] where all frequencies are included. For fixed truncated Hamiltonian , as N_{tr} increases, α_c converges to the true value from above very quickly. We believe that we obtain the converging critical points for any values of Δ for fixed N in the present work.

The ground-state fidelity susceptibility χ is defined as the second derivative of the fidelity [21, 23]

$$\chi(\alpha) = 2 \lim_{\delta\alpha\to 0} \frac{1 - F(\alpha, \delta\alpha)}{\delta\alpha^2}. \tag{15}$$

Since χ is independent of the arbitrary small parameter $\delta\alpha$, it is regarded as a more effective tool to detect the singularity in QPT. As addressed in Ref. [23], the fidelity susceptibility is similar to the magnetic susceptibility. In the localized phase, the scaling behavior of fidelity susceptibility χ obeys

$$\chi(\alpha) \propto |\alpha - \alpha_c|^{\beta} \tag{16}$$

Recently, the studies from the QMC approach[15], the exact-diagonalization [16], and the modified NRG[17] have shown that the quantum-to-classical mapping is valid for the sub-Ohmic spin-boson model, i.e. the critical exponents are classical, mean-field like, in contrast with the early standard NRG calculations where the quantum-to-classical mapping is suggested to fail for $s < 1/2$. It was argued [15] that the standard NRG is not able to capture the correct physics in the localized phase. It is known that the localized phase is two-fold degenerate. Our ansatz Eqs. (7-10) is just proposed for these two states, and the unknown coefficients can be obtained by solving the Schrödinger equations very accurately. Therefor, we will extract the susceptibility critical exponent for $s < 1/2$, to address this crucial controversy.

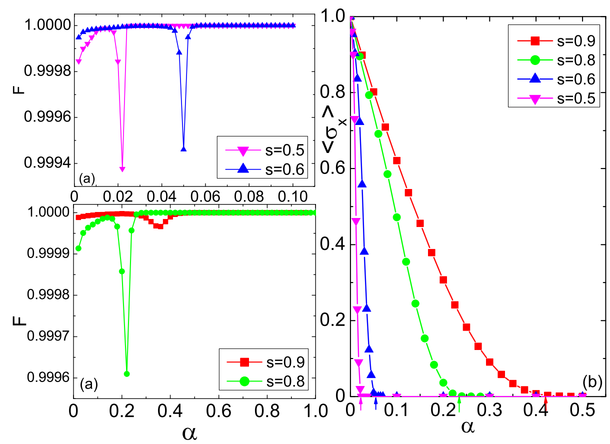

FIG. 1: (Color online). (a) The fidelity F as a function of α for various values of s and (b) The tunneling $\langle\sigma_x\rangle$ between two states of the spin as a function of α in the case of $\Delta = 0.01$ and $\epsilon = 0$..

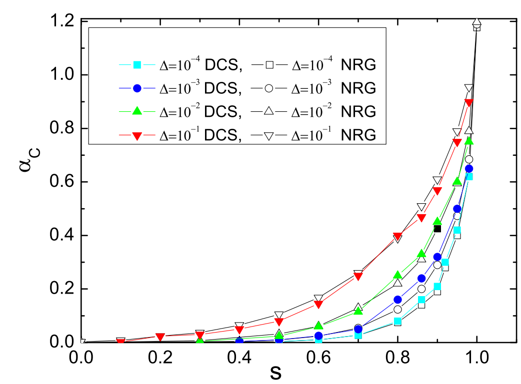

FIG. 2: (Color online). The delocalized-localized transition point α_c as functions of s obtained by the present approach in the case $\Delta = 10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}$. The NRG data are also shown for comparison.

Fig. 3 presents that the fidelity susceptibility χ as a function $(\alpha - \alpha_c)$ for $s = 0.1, 0.2, 0.3, 0.4$ in log-log scale. All curves show almost perfect straight line with a slope very close to -1, demonstrating that the susceptibility critical exponent may be just equals to $\beta = -1$ with $\chi \sim (\alpha - \alpha_c)^{-1}$. Recently, the critical exponent of the magnetic susceptibility has been estimated to be -1 by

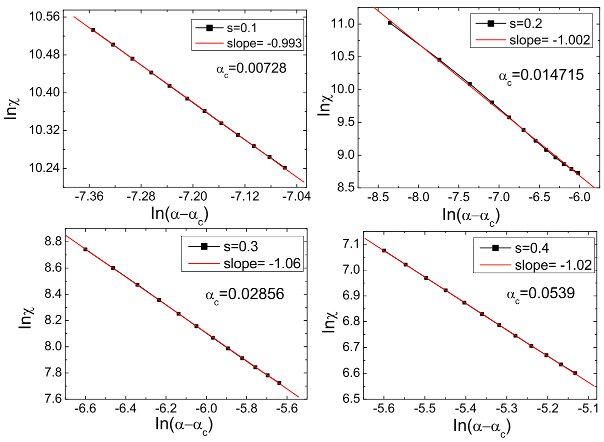

FIG. 3: (Color online). The scaling behavior of the fidelity susceptibility $\chi \sim |\alpha - \alpha_c|^{\beta}$ in log-log scale for $s = 0.1, 0.2, 0.3, 0.4$ with $\Delta = 0.1$. The data fit well with the straight line with slope very close to -1.

QMC simulations [15] and exact-diagonalization studies [16]. We do not think this is a coincidence. You et al [23] have shown a neat connection between the fidelity susceptibility χ and the magnetic susceptibility χ_m through $\chi = \chi_m/4K_BT$ (K_B is the Boltzmann constant, T is the temperature). We believe this relation is also applicable to zero temperature, and therefore these two susceptibilities can give the same order-parameter critical exponents in QPT. We also confirm the mean-field behavior for $1/2 < s < 1$.

In summary, we have introduced an efficient algorithm in the new bosonic coherent Hilbert space and presented reliable solution for the sub-Ohmic spin-boson model. The ground-state fidelity, which is a quantum information tool, is employed to locate the critical coupling strength α_c of the QPT . The transition from the localized phase to delocalized phase is accompanied by a minimum of the fidelity. Furthermore, the fidelity susceptibility gives the order-parameter critical exponent $\beta = -1$ in the case $s < 1/2$, which agrees well with the exponent of magnetic susceptibility. Both behaviors of the tunneling $\langle \sigma_x \rangle$ and the fidelity around the critical point exclude the possibility of the first-order QPT. We stress that all eigenstates and eigenvalues of the spin-boson model can be obtained accurately and many observable can be calculated directly within the present approach. The present technique to deal with bosons would be combined with other established methods.

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